Systematics of the first 2^+ excitation with the Gogny interaction

G.F. Bertsch[1], M. Girod[2], S. Hilaire[2], J.-P. Delaroche[2], H. Goutte[2] and S. Péru[2]
[1] *Department of Physics and Institute of Nuclear Theory, Box 351560 University of Washington Seattle, WA 98915 USA*
[2] *CEA/DAM Ile de France, DPTA/Service de Physique Nucléaire, BP 12, 91680 Bruyères-le-Chatel, France*

We report the first comprehensive calculations of 2^+ excitations with a microscopic theory applicable to over 90% of the known nuclei. The theory is based on a quantal collective Hamiltonian in five dimensions in which the potential energy and the tensor of inertia are obtained from constrained triaxial Hartree-Fock-Bogoliubov calculations. The only parameters in theory are those of the finite-range, density-dependent Gogny D1S interaction. The following properties of the lowest 2^+ excitations are calculated: excitation energy, reduced transition probability, and spectroscopic quadrupole moment. 519 nuclei are included in our survey, comprising all but 38 of the known nuclei tabulated by Raman et al. [1]. We find that the theory is very reliable to classify the nuclei by shape. Quantitatively the performance of the theory in deformed nuclei is excellent: average excitation energies and transition quadrupole moments are within 5% of the experimental values, and the dispersion about the averages are roughly 20% and 10%, respectively. The performance is not as good on spherical and soft nuclei. Including all nuclei in the performance evaluation, the average transition quadrupole moment is 11% too high and the dispersion about the mean is $\sim 20\%$. For the energies, the average is 13% too high and the dispersion is $\sim 40\%$.

I. INTRODUCTION

A framework for a comprehensive theory of nuclear structure has been discussed for a long time [2], but up to now there has been no systematic evaluation of the accuracy or reliability of different methods used and their underlying energy functionals. Methodologies based on self-consistent mean field theory or density functional theory have been extended in different ways with many of their details dependent on the energy functional's form. Except for one new study [3], the extensions to treat properties of excited states have been tested only in limited regions of nuclei. In this work we examine the properties of the lowest 2^+ excited state over the periodic table as a whole, using a methodology and energy functional that has been quite successful in previous studies of strongly deformed nuclei [5, 6, 7] and soft nuclei [8, 9].

The present theory uses the Generator Coordinate Method with the Gaussian Overlap Approximation (GCM+GOA) to construct a collective Hamiltonian. The elements of the theory are well-known in nuclear physics [2]. One starts with the Constrained Hartree-Fock-Bogoliubov (CHFB) theory of the potential energy surface, and constructs a collective Hamiltonian from the potential energy surface and the information about the kinetic energy operator obtained from the wave functions on that surface. The finite-range density-dependent Gogny interaction D1S is used throughout; the only parameters in the theory are those of D1S [10, 11]. The microscopic collective Hamiltonian (5DCH) is formally similar to the Bohr Hamiltonian. It has six kinetic terms, associated with three rotational moments of inertia and three mass parameters stemming from the fluctuations of axial and triaxial deformations. The rotational moments of inertia are obtained using the Thouless-Valatin prescription from the CHFB solutions in the presence of a small rotational field. We emphasize that there are no adjusted parameters in the present treatment of the rotational moments of inertia. The mass parameters are calculated by the Inglis-Belyaev formula, which only requires local information about the CHFB solutions on the grid points of a mesh in deformation space. This is sufficient information to construct the collective Hamiltonian, but not enough to compute matrix elements. For that, one needs the overlaps between states of different deformations. This is also computed using a local approximation [5]. The local approximations are quite accurate for heavy open shell nuclei, but break down when applied to doubly magic nuclei, because the overlap between CHFB states is not sharp enough [2]. We therefore exclude those nuclei from this study. The properties we discuss are the excitation energy E, the transition quadrupole moment $\langle 2||\hat{Q}_2||0\rangle$ between the ground and the excited states, and the spectroscopic quadrupole moment $Q(2^+)$ of the excited state.

II. RESULTS

There are 557 even-even nuclei with known 2^+ excitation energies as of compilation by Raman *et al.* in 2001 [1]. Their excitation energies span more than two orders of magnitude, presenting a very substantial challenge to any global theory of nuclear structure. In our study here we limit our scope somewhat by excluding the very light nuclei (Z or $N < 8$), for which mean field theory is least justified. This eliminates 16 nuclei. Also, the mapping of the CHFB to the collective Hamiltonian becomes prob-

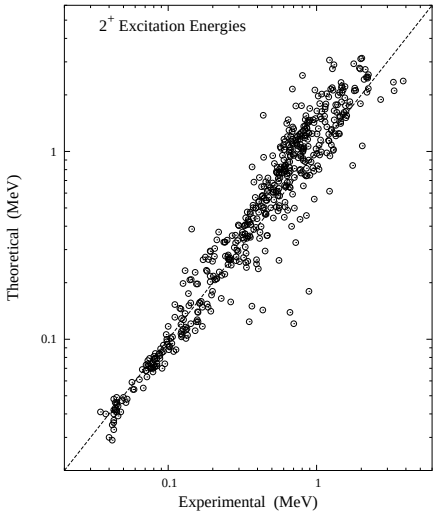

FIG. 1: Scatter plot of 519 even-even nuclei as a function of their experimental and theoretical 2^+ excitation energies.

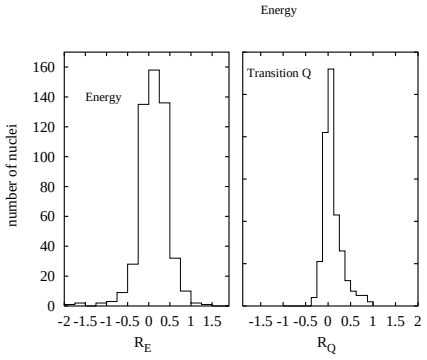

FIG. 2: Histogram of the logarithmic errors R_E, R_Q of the present theory. Left panel: energies of the first excited 2^+ states for 519 of the 557 nuclei whose excitation energies are tabulated in ref. [1]; right panel: matrix elements $\langle 2||\hat{Q}_2||0\rangle$ for the transition between the ground and first excited state for 318 of the 328 nuclei whose $B(E2)$ values are tabulated in ref. [1].

lematic for rigid spherical nuclei such as the doubly magic ones. An additional 23 nuclei have been eliminated for that reason, leaving 519 nuclei in the present study. We first discuss the energies and then the quadrupole properties of the nuclei

A. Excitation energies

Fig. 1 shows a scatter plot comparing experimental and theoretical excitation energies. The points follow the diagonal line fairly well with some scatter that varies in extent over the different excitation energy regimes. The lowest energies are for the heavy, strongly deformed actinide nuclei; the theoretical energies here are the most accurate (on a logarithmic as well as absolute scale). At excitation energies of 1 MeV and higher, the theory has only a qualitative predictive power, with errors ranging to a factor of 2 and larger. In the middle the theory improves but one can see a few nuclei far from the diagonal. They correspond to neutron-deficient isotopes of Hg and Pb, where there is a near-degeneracy of weakly deformed oblate and well-deformed prolate structures.

To make a quantitative measure of the theoretical accuracy, we compare theory and experiment on a logarithmic scale, examining the statistical properties of the quantity $R_E = \log(E_{\rm th}/E_{\rm exp})$. Here $E_{\rm th}$ and $E_{\rm exp}$ are the theoretical and experimental excitations energies, respectively. A histogram of distribution of the R_E's is shown in Fig. 2. One can see that there is a bias to positive values of R_E, i.e. an overprediction of the excitation energy. For the set of 519 nuclei, the average is $\bar{R}_E = 0.12$. Thus, there is a systematic bias to overestimate the excitation energy by 12%.

The width of the distribution is the important quantity to determine the accuracy and reliability of the theory. One can see from the histogram that the peak in the distribution extends from R_E about -0.25 to +0.50, with a small tail going much farther from zero. A single number cannot be adequate to express the width of such a distribution, but for purposes of future comparisons with other theories we report the root mean square deviation of R_E about its mean. This measure comes out to $\sigma_E \equiv \langle \Delta R_E^2 \rangle^{1/2} = 0.33$. This implies that typical errors are around -30% on the low side to +40% on the high side after correcting for the systematic bias. While these results may seem disappointing, one should remember that present predictions are from a global theory with no parameter adjustment.

B. Quadrupolar properties

The compilation of Raman *et al.* includes 328 measured quadrupole transition rates. Of these, 318 met the conditions for applying the 5DCH theory. The comparison between theoretical and experimental reduced transition rates $B(E2, 0^+ \rightarrow 2^+)$ are shown as a scatter plot in Fig. 3. One sees that the theory is quite accurate for the largest values; these are the actinide nuclei which are both heavy and strongly deformed.

For a quantitative measure of the accuracy of the theory, we define $R_Q = \log\left(\langle 2||\hat{Q}_2||0\rangle_{th}/\langle 2||\hat{Q}_2||0\rangle_{exp}\right)$, the logarithm of the ratio of the transition matrix elements. The distribution of R_Q values is plotted as a histogram in the right panel of Fig. 2. We see that the distribution is narrow and centered close to zero. The average of R_Q values is 0.10, corresponding to a matrix elements 11% too large on average. The dispersion σ_Q is 0.21, corresponding to a range of $+20/-19$ % about the center value.

Next we examine the spectroscopic quadrupole moments of the first excited 2^+ states. The comparison with experiment for 98 nuclei is shown in Fig. 4 on lin-

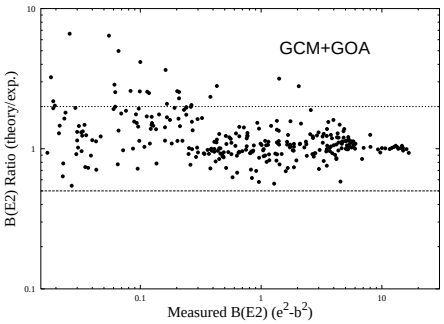

FIG. 3: Experiment compared to theory for the $B(E2, 0^+ \rightarrow 2^+)$ for the nuclei tabulated in ref. [1]. This graph may be directly compared with their Fig. C. Values within the lines are within a factor of two of experiment. Of the 306 cases shown here, 93% are within the error band. This is superior to their "GLOBAL" phenomenological fit and is much better than the theoretical models they consider.

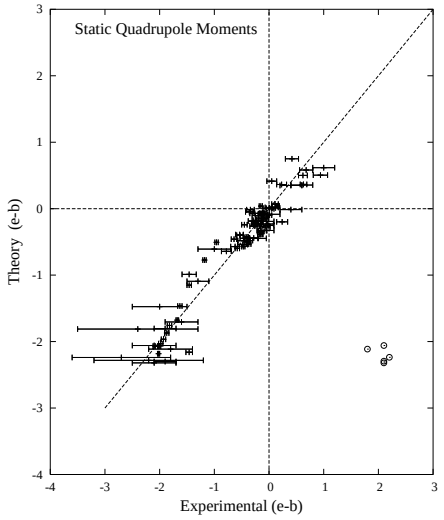

FIG. 4: Experiment compared to theory for the quadrupole moment of 98 excited 2^+ states. Experimental database is from the tabulation in ref. [12].

ear scales. For the experimental data, we have used the tabulation by Stone in ref. [12]. The quality of the experimental information is quite variable, and we present only the cases where the assigned error was much smaller than the magnitude of the moment. Even so, there are cases (^{160}Dy, ^{170,174,176}Yb and ^{180}W) in which the sign of the moment is not determined. These nuclei appear on the graph twice: once with error bars, assuming that the theory gives the correct sign, and once with open circles, assuming the opposite sign. They are all predicted to be prolate with an negative quadrupole moment. Globally, there is a very good agreement between $Q(2^+)$ measurements and predictions.

III. PERFORMANCE BY NUCLEAR TYPE

It is clear that the 5DCH theory performs much better for strongly deformed nuclei than for spherical ones. To make this observation quantitative, we attempted to sort the nuclei into different categories and evaluate the $R_{Q,E}$ statistics by category. To make this as systematic as possible, we define the categories on the basis of the theoretical properties of the nuclei. Thus, no empirical data is used to select the most favorable cases.

The most obvious way to define a strongly deformed nucleus is to make a cut on the mean quadrupole deformation $\bar{\beta}$. However, if the cut is at large enough $\bar{\beta}$ to include the well-known deformed nuclei in the rare earths and actinides, it will also keep certain light nuclei that have large mean $\bar{\beta}$ as well as strong fluctuations in $\bar{\beta}$. We therefore adopt the classification by Sabbey, et al. [3], defining a strongly deformed nucleus as one in which the mean deformation $\bar{\beta}$ is larger than the r.m.s. fluctuation in $\bar{\beta}$. We also define a category "semimagic" in which either the proton or neutron number has the value $8, 20, 28, 50, 82,$ or 126. The remaining nuclei in our study can be considered either spherical or soft-deformed; they are lumped together in the category "other". The $R_{Q,E}$ statistics by category are given in Table I. One sees that the bias in average energy depends on the category: deformed nuclei are slightly unpredicted, the "other" category are overpredicted, and the semimagic nuclei are correct on average. However, the dispersions in categories except the deformed one are large. Here the semimagic nuclei are the poorest, with the theory too high on average by almost 50 %. In the bottom half of the Table, for the reduced matrix elements, the entry for the deformed nuclei stands out with an average of 0.035 and a dispersion of less that 0.1.

TABLE I: Statistics for the performance of the 5DCH theory using the Gogny D1S interaction on properties of 2^+ excitations. The quantities $\bar{R}$ and σ are defined in the text.

Category	Number of Nuclei	$\bar{R}$	σ
Excitation Energy			
All	519	0.12	0.33
Semimagic	73	0.02	0.51
Deformed	146	-0.05	0.19
Other	300	0.22	0.29
$\langle 2\|\|\hat{Q}_2\|\|0\rangle$			
All	319	0.10	0.21
Semimagic	43	0.42	0.23
Deformed	106	0.035	0.09
Other	170	0.065	0.19

IV. CONCLUSION

In this work we have tested a theory of nuclear structure with respect to the properties of the lowest 2^+ excitations in even-even nuclei. The theory is the microscopic collective Hamiltonian for quadrupole degrees of freedom in which all parameters are determined by CHFB input using the Gogny D1S interaction. The CHFB starting point imposes shell characteristics on the nuclear structure, and this persists to a considerable extent in the collective Hamiltonian. The 5DCH theory is quite reliable for open proton and neutron shell nuclei. Here there are strong correlations that break the naive shell picture and often reorganize the wave functions into a deformed band with distinctive signatures in the properties of the first 2^+ excitation. For nuclei having only one open shell the theory is still useful for predicting excitation energies and quadrupole transition moments–much better than a factor 2–but one does not achieve the quantitative, 10%-level accuracy that we found for the deformed nuclei. Finally, in doubly closed shell nuclei, the mapping of CHFB to the collective Hamiltonian breaks down and the theory cannot be used. Still, we found that the calculations could be made applying the theory to more than 90 % of the nuclei whose 2^+ excitations are known.

For future work, the good results for deformed nuclei is encouraging to a global study of other excitations implied by the 5DCH. In particular, softness in the axial and triaxial coordinates β and γ gives rise to low-lying vibrations. The γ vibrations appear as higher lying 2^+ excitations, and the systematics of their energies and transition quadrupole moments would provide a severe test of the 5DCH theory. The β vibration appears as 0^+ excitation on top of which is built a rotational band; besides its energy in many cases its monopole transition matrix element to the ground state is known.

Concerning the methodology, there are many points that need more theoretical attention. A weak point in the present study is the Inglis-Belyaev approximation for the collective masses. A better approximation would be that based on the QRPA theory [2]. The same theory is also suitable for the prediction of collective and non-collective modes in closed shell nuclei for which the GCM+GOA theory may break down. Such works are in progress.

A systematic study of 2^+ state energies has also been performed recently by Sabbey et al. [3] using a different energy functional and methodology. There i) the zero-range Skyrme force is used in Hartree-Fock+BCS mean field calculations restricted to axial quadrupole deformation; ii) the configurations generated by the GCM are projected on angular momentum J = 0 and 2 and good particle numbers; iii) the configuration mixing is carried out directly rather than through a collective Hamiltonian. In principle that method is applicable to all nuclei including the doubly magic, but they only reported results for two-thirds of the measured nuclei, due to numerical difficulties associated with the discrete basis.

Their theory does very well on the quadrupole properties of deformed nuclei, showing that this aspect of nuclear structure is robust in self-consistent mean-field theory. However, their calculated energies are systematically higher than ours and higher than the data by about 50%. At this time it is not clear what the origin of the difference is. Certainly, the dependence on the functionals and on the theoretical approximations needs to be investigated further.

Acknowledgment

This work was supported in part by the Department of Energy Grants DE-FG02-00ER41132 and DE-FC02-07ER41457.

[1] S. Raman, C. W. Nestor, Jr., and P. Tikkanen, At. Data Nucl. Data Tables **78**, 1 (2001); the 2^+ excitation energy of ^{114}Ru has been corrected to the value given in ref. [4].
[2] P. Ring, P. Schuck, The Nuclear Many-Body Problem, Springer-Verlag, New York (1980) p. 424.
[3] B. Sabbey, M. Bender, G.F. Bertsch, and P.-H. Heenen, Phys. Rev. C **75** 044305 (2007).
[4] J.A. Shannon, et al., Phys. Lett. B336 136 (1994).
[5] J. Libert, M. Girod, and J.-P. Delaroche, Phys. Rev. C60 054301 (1999).
[6] JP Delaroche, et al., Nucl. Phys. A771 103 (2006).
[7] H. Goutte,J.-F. Berger, P. Casoli, and D. Gogny, Phys. Rev. C71 024316 (2005).
[8] W. Boeglin et al., Nucl. Phys. A477 (1988) 399.
[9] P. Fleischer, P. Klüpfel, P.-G. Reinhard, and J. A. Maruhn, Phys. Rev. C **70** (2004) 054321.
[10] J. Dechargé, D. Gogny, Phys. Rev. C 21 (1980) 1568.
[11] J.-F. Berger, M. Girod, D. Gogny, Comp. Phys. Comm. 63 (1991) 365.
[12] N.J. Stone, At. Data Nucl. Data Tables **90** 75 (2005).